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THE WIGNER DISTRIBUTION FUNCTION

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In this letter, the relationship between the characteristic function for two arbitrary noncommuting observables and a generalized Wigner distribution function is established. This distribution function is shown to have no simple interpretation in the sense of probability theory but, in lieu of its special properties, can be used directly for calculating the expectation values of observables.

Whereas classical transport physics is based on the concept of a probability distribution function which is defined over the phase space of the system, in the quantum formulation of transport physics, the concept of a phase space distribution function is not possible inasmuch as the noncommutation of the position and momentum operators (the Heisenberg uncertainty principle) precludes the precise specification of a point in phase space. However, within the matrix formulation of quantum mechanics, it is possible to construct a "probability" density matrix which is often interpreted as the analog of the classical distribution function.

There is yet another approach to the formulation of quantum transport, based on the construction of the Wigner distribution function [1]. As we shall show, this distribution function has no simple interpretation in the sense of probability theory [2] but, in lieu of its special properties, can be used directly for calculating expectation values [3–5] of observables in a manner quite analogous to that of classical theory, i.e. by integrating the product of the observable and the Wigner distribution function over all phase space.

This letter, in part, reviews the salient features of the Wigner distribution function. Although the Wigner function is generally defined in terms of all the generalized coordinates and momenta of the system in question as

$$P_W(x_1 \dots x_n, p_1 \dots p_n) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dy_1 \dots dy_n \times \Psi^*(x_1 + \tfrac{1}{2}y_1, \dots x_n + \tfrac{1}{2}y_n) \times \Psi(x_1 - \tfrac{1}{2}y_1, \dots x_n - \tfrac{1}{2}y_n) \times \exp[i(p_1 y_1 + \dots + p_n y_n)/\hbar] , \quad (1)$$

we will discuss the properties of the Wigner function in terms of a single coordinate and momentum. In this case, we let

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$$P_W(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dy\, \Psi^*(x+\tfrac{1}{2}y)\Psi(x-\tfrac{1}{2}y)e^{ipy/\hbar}, \tag{2}$$

where $\Psi(x)$ refers to the state of the system in the coordinate representation.

The distribution function of eq. (2) has interesting properties in that the integration of this function over all momenta leads to the probability density in real space; conversely, the integration of this function over all coordinates leads to the probability density in momentum space. In mathematical terms,

$$\int_{-\infty}^{\infty} P_W(x,p)\,dp = \Psi^*(x)\Psi(x) \tag{3a}$$

and

$$\int_{-\infty}^{\infty} P_W(x,p)\,dx = \phi^*(p)\phi(p), \tag{3b}$$

where

$$\phi(p) = (2\pi\hbar)^{-1/2}\int_{-\infty}^{\infty} e^{-ipx/\hbar}\Psi(x)\,dx .$$

It follows immediately from eq. (3) that, for an observable $W(x,p)$ which is either a function of momentum operator alone or of position operator alone, or any additive combination therein, the expectation value of the observable is given by

$$\langle W\rangle = \iint W P_W(x,p)\,dx\,dp , \tag{4}$$

which is analogous to the classical expression for the average value. Herein lies the interesting aspect of the Wigner distribution function; the result of eq. (4) suggests that it is possible to transfer many of the results of classical transport theory into quantum transport theory by simply replacing the classical distribution function by the Wigner distribution function. However, unlike the density matrix, the Wigner distribution function itself cannot be viewed as the quantum analog of the classical distribution function since it is generally not positive definite and nonunique [$P_W(x,p)$ of eq. (2) is not the only bilinear expression [1,3–5] in Ψ that satisfies eq. (3)].

Further resemblance of the Wigner distribution function to the classical distribution function is apparent by examining the equation of time evolution for $P_W(x,p)$. Upon assuming that $\Psi(x)$ in eq. (2) satisfies the Schrödinger equation for a system with hamiltonian $H = p^2/2m + V(x)$, it can be readily shown that $P_W(x,p)$ satisfies the equation

$$\partial P_W/\partial t + (p/m)\,\partial P_W/\partial x + \theta\cdot P_W = 0 , \tag{5}$$

where

$$\theta\cdot P_W = -\frac{2}{\hbar}\sum_{n=0}^{\infty}(-1)^n\frac{(\hbar/2)^{2n+1}}{(2n+1)!} \times \frac{\partial^{2n+1}V(x)}{\partial x^{2n+1}}\,\frac{\partial^{2n+1}P_W(x,p)}{\partial p^{2n+1}}. \tag{6}$$

It is evident that in the limit $\hbar\to 0$, $\theta\cdot P_W$ in eq. (6) becomes

$$\theta\cdot P_W = -(\partial V/\partial x)(\partial P_W/\partial p) \tag{7}$$

so that eq. (5) reduces to the classical collisionless Boltzmann equation.

The Wigner distribution function defined in eq. (2) is derivable [6] from the Fourier inversion of the expectation value (with respect to state $\Psi(x)$ of the operator $e^{i(\tau\hat{p}+\theta\hat{x})}$ (here, $\hat{x}$ and $\hat{p}$ satisfy the commutation relation $[\hat{x},\hat{p}] = i\hbar$). As such,

$$P_W(x,p) = \frac{1}{4\pi^2}\iint C_W(\tau,\theta)e^{-i(\tau p+\theta x}d\tau\,d\theta , \tag{8a}$$

where

$$C_W(\tau,\theta) = \int \Psi^*(x)e^{i(\tau\hat{p}+\theta\hat{x})}\Psi(x)\,dx , \tag{8b}$$

and the interval of integration is $(-\infty,\infty)$ unless otherwise specified. In order to show that the right-hand side of eq. (8a) is indeed the Wigner distribution function as defined in eq. (2), note, from the Baker–Hausdorff theorem [7], that $e^{i(\tau\hat{p}+\theta\hat{x})}$ can be written as

$$e^{i(\tau\hat{p}+\theta\hat{x})} = e^{i\tau\hat{p}/2}e^{i\theta\hat{x}}e^{i\tau\hat{p}/2} , \tag{9}$$

in which case $C_W(\tau,\theta)$ of eq. (8b) becomes

$$C_W(\tau,\theta) = \int_{-\infty}^{\infty}[e^{-i\tau\hat{p}/2}\Psi(x)]^* e^{i\theta\hat{x}}[e^{-i\tau\hat{p}/2}\Psi(x)]\,dx , \tag{10}$$

which further reduces to

$$C_W(\tau,\theta)=\int_{-\infty}^{\infty}\Psi^*(x-\tfrac{1}{2}\tau h)e^{i\theta x}\Psi(x+\tfrac{1}{2}\tau h)\,dx\,. \quad (11)$$

Then, by inserting $C_W(\tau,\theta)$ of eq. (11) into the right-hand side of eq. (8a), integrating over the variable θ by using the relation

$$\int_{-\infty}^{\infty}e^{i\theta(x'-x'')}\,d\theta=2\pi\delta(x'-x'')\,,$$

and letting $\tau=-y/h$, the desired result is obtained.

The method outlined above to arrive at the Wigner distribution function is based on the notion of a characteristic function. The characteristic function of an observable, A, with respect to state $|\Psi\rangle$ (here, the Dirac notation is utilized for purposes of generality) is defined as

$$C_A(\xi)=\langle\Psi|e^{i\xi\hat{A}}|\Psi\rangle\,, \quad (12)$$

where ξ is a real parameter. Assuming $\hat{A}$ to possess an eigenvalue spectrum given by $\hat{A}|A'\rangle=A'|A'\rangle$, $C_A(\xi)$ can be evaluated in the A'-representation as

$$C_A(\xi)=\int dA'\int dA''\langle\Psi|A'\rangle\langle A'|e^{i\xi\hat{A}}|A''\rangle\langle A''|\Psi\rangle\,. \quad (13)$$

Since $\langle A'|e^{i\xi\hat{A}}|A''\rangle=e^{i\xi A'}\delta(A'-A'')$ in the A'-representation, $C_A(\xi)$ in eq. (13) reduces to

$$C_A(\xi)=\int dA' e^{i\xi A'}|\Psi_{A'}|^2\,, \quad (14)$$

where $|\Psi_{A'}|^2=|\langle A'|\Psi\rangle|^2\equiv P(A')$, the probability distribution function for measuring A' while in state $|\Psi\rangle$. Hence, the characteristic function for $\hat{A}$ is the Fourier transform of the probability distribution function $P(A')$. Subsequent inversion of eq. (14) above leads to

$$P(A')=\frac{1}{2\pi}\int C_A(\xi)e^{-i\xi A'}\,d\xi\,. \quad (15)$$

The Wigner distribution function was derived by taking the Fourier transform of the characteristic function for $e^{i(\tau\hat{p}+\theta\hat{x})}$. In view of the connection between the probability distribution function and the characteristic function for a given observable, this approach seems to be a natural way of obtaining a distribution function for momentum and position. Unfortunately, the noncommutative nature of the two observables destroys the convenient probability interpretation of the characteristic function implicit in eq. (15).

In order to demonstrate this point, assume the characteristic function for two noncommuting observables, $\hat{A}$ and $\hat{B}$, to be

$$C_{AB}(\xi_1\xi_2)=\langle\Psi|e^{i(\xi_1\hat{A}+\xi_2\hat{B})}|\Psi\rangle\,. \quad (16)$$

Observables $\hat{A}$ and $\hat{B}$ are assumed to have eigenvalue spectra

$$\hat{A}|A'\rangle=A'|A'\rangle\,,\quad \hat{B}|B'\rangle=B'|B'\rangle\,, \quad (17)$$

and are chosen so that $[\hat{A},[\hat{A},\hat{B}]]=[\hat{B},[\hat{A},\hat{B}]]=0$. This assumption is imposed so that the identity

$$e^{i(\xi_1\hat{A}+\xi_2\hat{B})}=e^{i\xi_1\hat{A}}\,e^{i\xi_2\hat{B}}\,e^{-\xi_1\xi_2[\hat{A},\hat{B}]/2} \quad (18)$$

may be used.

Inserting eq. (18) into eq. (16) while obtaining the matrix elements of $e^{i\xi_1\hat{A}}$ in the A'-representation and $e^{i\xi_2\hat{B}}$ in the B'-representation results in

$$C_{AB}(\xi_1\xi_2)=e^{-\xi_1\xi_2[\hat{A},\hat{B}]/2}\int dA'\int dB' \times e^{i(\xi_1A'+\xi_2B')}\langle\Psi|A'\rangle\langle A'|B'\rangle\langle B'|\Psi\rangle\,. \quad (19)$$

In eq. (19), it is assumed that $[\hat{A},\hat{B}]$ is a c-number independent of the eigenvalues A' and B'. We define $F(A',B')$, the generalized Wigner distribution function [‡1], to be

$$F(A',B')=\langle\Psi|A'\rangle\langle A'|B'\rangle\langle B'|\Psi\rangle\,, \quad (20)$$

so that

$$F(A',B')=\frac{1}{(2\pi)^2}\int d\xi_1\int d\xi_2\, e^{\xi_1\xi_2[\hat{A},\hat{B}]/2} \times C_{AB}(\xi_1,\xi_2)e^{-i(\xi_1A'+\xi_2B')}\,. \quad (21)$$

It is evident from eqs. (20,21) that

[‡1] The form of the generalized distribution function derived is sensitive to the manner in which $\exp[i(\xi_1\hat{A}+\xi_2\hat{B})]$ is expanded. For example, if instead of eq. (18), we used the forms $\exp(i\xi_2\hat{B})\exp(i\xi_1\hat{A})\exp(\xi_1\xi_2[\hat{A},\hat{B}]/2)$, $\exp(i\xi_1\hat{A}/2)\times\exp(i\xi_2\hat{B})\exp(i\xi_1\hat{A}/2)$, or $\exp(i\xi_2\hat{B}/2)\exp(i\xi_1\hat{A})\exp(i\xi_2\times B/2)$, all of which are equivalent, we would indeed obtain a different form of the generalized distribution function, yet one which obeys the sum rules of eq. (22).

$$\int F(A',B')\,dA' \equiv |\langle B'|\Psi\rangle|^2 = \frac{1}{2\pi}\int d\xi_2 \times C_{AB}(0,\xi_2)\,e^{-i\xi_2 B'} \tag{22a}$$

and

$$\int F(A',B')\,dB' \equiv |\langle A'|\Psi\rangle|^2 = \frac{1}{2\pi}\int d\xi_1 \times C_{AB}(\xi_1,0)\,e^{-i\xi_1 A'} . \tag{22b}$$

Thus, eq. (21) establishes the relationship between the characteristic function for two arbitrary noncommuting observables and the generalized Wigner distribution function. The generalized distribution function has the essential properties of the conventional Wigner function in that an integration of the generalized function over the eigenvalue spectrum of one observable leads to the probability density in the canonically conjugate observable [eq. (22)].

There is no simple probability interpretation of $F(A',B')$ in eqs. (20, 21) because of the necessary overlap between the states of the noncommuting observables. However, if $\hat{A}$ and $\hat{B}$ are made to commute so that $|A'\rangle$ and $|B'\rangle$ are a common set of eigenvectors, then $F(A',B')$ reduces to the probability distribution function for $\hat{A}$ and $\hat{B}$.

Finally, it is noted that the conventional Wigner distribution function for observables $\hat{A}$ and $\hat{B}$ is obtained from

$$P_W(A',B') = \frac{1}{(2\pi)^2}\int d\xi_1 \int d\xi_2 \times C_{AB}(\xi_1,\xi_2)\,e^{-i(\xi_1 A' + \xi_2 B')} , \tag{23}$$

with $C_{AB}(\xi_1\xi_2)$ defined in eq. (16), whereas the alternative distribution function, $F(A',B')$, introduced in eqs. (20, 21) differs from the Wigner function due to the presence of the phase factor $e^{\xi_1\xi_2[\hat{A},\hat{B}]/2}$ in the integrand of eq. (21). For $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$, $P_W(x,p)$ in eq. (23) reduces to the Wigner function of eq. (2), whereas $F(x,p)$ defined from eq. (20) becomes

$$F(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dy\, \Psi^*(x)\Psi(x-y)\,e^{ipy/\hbar} \equiv (2\pi\hbar)^{-1/2}\,\Psi^*(x)\,e^{ipx/\hbar}\,\phi(p) , \tag{24}$$

where $\phi(p)$ is defined in eq. (3b). It is evident that there is a family of functions which are bilinear in Ψ yet satisfy the sum rules of eqs. (3a, b).

There are some interesting questions to be resolved concerning the uniqueness and positive definiteness of Wigner-type quantum distribution functions. Nevertheless, these distribution functions serve a useful purpose for calculating quantum mechanical observables in transport [5] studies and numerous solid-state [8,9] problems.

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